The `phylo4` S4 classes and methods

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1 Introduction

This document describes the new `phylo4` S4 classes and methods, which are intended to provide a unifying standard for the representation of phylogenetic

trees and comparative data in R. The `phylobase` package was developed to help both end users and package developers by providing a common suite of tools likely to be shared by all packages designed for phylogenetic analysis, facilities for data and tree manipulation, and standardization of formats.

For *end-users*, standardization will greatly simplify comparing analyses across different packages by easing data portability, as well as reducing the learning curve involved when using new packages. Users will also benefit by having a common repository of useful functions contained within one base package, for example tools for including or excluding subtrees (and associated phenotypic data) or improved tree and data plotting facilities. For *developers*, the `phylobase` package allows programming efforts to be put directly into developing new solutions for new problems (i.e. new phylogenetic methods) rather than re-coding the same base tools that each package requires. It is hoped that standardization will also synergize the efforts of individual developers into a comparative method community (this sounds stupid– please fix), as well as facilitating code validation by providing a repository for benchmark tests.

On a more abstract level, two motivations for the development of this package were better data checking and abstraction of the tree data formats. Currently `phylobase` is capable of checking that data and trees are associated in the proper fashion, and protects users and developers from accidently reordering one, but not the other. The `phylobase` package also seeks to abstract the data format so that commonly used information (for example, branch length information or the ancestor of a particular node) can be accessed without knowing the underlying data structure (i.e., whether the tree is stored as a matrix, or a list, or a parenthesis-based format). This is achieved through generic `phylobase` functions which which retrieve the relevant information from the data structures. The benefits of such abstraction are multiple: (1) *easier access to the relevant information* via a simple function call (this frees both users and developers from learning details of complex data structures), (2) *freedom to optimize data structures in the future without breaking code.* Having the generic functions in place to "translate" between the data structures and the rest of the program code allows program and data structure development to proceed somewhat independently. The alternative is code written for specific data structures, in which modifications to the data structure requires rewriting the entire package code (often exacting too high a price, which results in the persistence of less-optimal data structures). (3) *providing broader access to the range of tools in* `phylobase`. Developers of specific packages can use these new tools based on S4 objects without knowing the details of S4 programming.

The base `phylo4` class is modeled on the the `phylo` class in `ape`. `phylo4d` and `multiphylo4` extend the `phylo4` class to include data or multiple trees respectively. In addition to describing the classes and methods this vignette gives examples of how they might be used.

2 Package Overview

The phylobase package currently implements the following functions and data structures:

- Data structures for storing a single tree and multiple trees: `phylo4` and `multiPhylo4`?
- A data structure for storing a tree with associated tip and node data: `phylo4d`
- A data structure for storing multiple trees with one set of tip data: `multiPhylo4d`
- Functions for reading nexus files into the above data structures
- Functions for converting between the above data structures and `ape phylo` objects as well as `ade4 phylog` objects
- Functions for editing trees and data (i.e., subsetting and replacing)
- Functions for plotting trees and trees with data

3 Using the S4 help system

The `S4` help system works similarly to the `S3` help system with some small differences relating to how `S4` methods are written. The `plot()` function is a good example. When we type `?plot` we are provided the help for the default plotting function which expects `x` and `y`. `R` also provides a way to smartly dispatch the right type of plotting function. In the case of an `ape phylo` object (a `S3` class object) `R` evaluates the class of the object and finds the correct functions, so the following works correctly.

```
> library(ape)
> rand_tree <- rcoal(10)
> plot(rand_tree)
```

However, typing `?plot` still takes us to the default `plot` help. We have to type `plot.phylo` to find what we are looking for. This is because `S3` generics are simply functions with a dot and the class name added.

The `S4` generic system is too complicated to describe here, but doesn't include the same dot notation. As a result `?plot.phylo4` doesn't work, `R` does, however, find the right plotting function.

```
> library(phylobase)
> rand_p4_tree <- as(rand_tree, "phylo4")
> plot(rand_p4_tree)
```

All fine and good, but how to we find out about all the great features of the phylobase plotting function? R has two nifty ways to find it, the first is to simply put a question mark in front of the whole call:

```
> ?plot(rand_p4_tree)
```

R looks at the class of the rand_p4_tree object and takes us to the correct help file (note: this only works with S4 objects). The second ways is handy if you already know the class of your object, or want to compare to generics for different classes:

```
> method?plot("phylo4")
```

More information about how S4 documentation works can be found in the methods package, by running the following command.

```
> help("Documentation", package = "methods")
```

4 Trees without data

You can start with a tree — an object of class phylo from the ape package (e.g., read in using the read.tree() or read.nexus() functions), and convert it to a phylo4 object.

For example, load the raw *Geospiza* data:

```
> data(geospiza_raw)
> names(geospiza_raw)
```

```
[1] "tree" "data"
```

Convert the S3 tree to a S4 phylo4 object using the as() function:

```
> library(phylobase)
> g1 <- as(geospiza_raw$tree, "phylo4")
> g1
```

```
          label node ancestor branch.length node.type
1           N01   15       NA            NA      root
2           N02   16       15       0.29744  internal
3           N03   17       16       0.04924  internal
4           N04   18       17       0.06859  internal
5           N05   19       18       0.13404  internal
6           N06   20       19       0.10346  internal
7           N07   21       20       0.03550  internal
8           N08   22       21       0.00917  internal
9           N09   23       22       0.07333  internal
10          N10   24       23       0.05500  internal
11          N11   25       19       0.24479  internal
```

```
12          N12   26       25       0.05167  internal
13          N13   27       26       0.01500  internal
14   fuliginosa    1       24       0.05500       tip
15       fortis    2       24       0.05500       tip
16 magnirostris    3       23       0.11000       tip
17  conirostris    4       22       0.18333       tip
18     scandens    5       21       0.19250       tip
19   difficilis    6       20       0.22800       tip
20      pallida    7       25       0.08667       tip
21     parvulus    8       27       0.02000       tip
22   psittacula    9       27       0.02000       tip
23       pauper   10       26       0.03500       tip
24   Platyspiza   11       18       0.46550       tip
25        fusca   12       17       0.53409       tip
26 Pinaroloxias   13       16       0.58333       tip
27     olivacea   14       15       0.88077       tip
```

Note that the nodes and edges are given default names if the tree contains no node or edge names.

The `summary` method gives a little extra information, including information on branch lengths:

```
> summary(g1)

  No root edge.

 Phylogenetic tree : g1

 Number of tips    : 14
 Number of nodes   : 13
 Branch lengths:
        mean         : 0.1764008
        variance     : 0.04624379
        distribution :
   Min. 1st Qu.  Median 3rd Qu.    Max.
0.00917 0.04985 0.08000 0.21910 0.88080
```

Print tip labels:

```
> labels(g1)

 [1] "fuliginosa"   "fortis"       "magnirostris" "conirostris"  "scandens"
 [6] "difficilis"   "pallida"      "parvulus"     "psittacula"   "pauper"
[11] "Platyspiza"   "fusca"        "Pinaroloxias" "olivacea"
```

Print internal node labels (R automatically assigns values):

```
> nodeLabels(g1)
```

```
 [1] "N01" "N02" "N03" "N04" "N05" "N06" "N07" "N08" "N09" "N10" "N11" "N12"
[13] "N13"
```

Print edge labels (also automatically assigned):

```
> edgeLabels(g1)
```

```
 [1] "E16" "E17" "E18" "E19" "E20" "E21" "E22" "E23" "E24" "E1"  "E2"  "E3"
[13] "E4"  "E5"  "E6"  "E25" "E7"  "E26" "E27" "E8"  "E9"  "E10" "E11" "E12"
[25] "E13" "E14"
```

Is it rooted?

```
> isRooted(g1)
```

```
[1] TRUE
```

Which node is the root?

```
> rootNode(g1)
```

```
[1] 15
```

Does it have any polytomies?

```
> hasPoly(g1)
```

```
[1] FALSE
```

Does it have branch lengths?

```
> hasEdgeLength(g1)
```

```
[1] TRUE
```

You can modify labels and other aspects of the tree — for example,

```
> labels(g1) <- tolower(labels(g1))
```

5 Trees with data

The `phylo4d` class matches trees with data. (**fixme: need to be able to use ioNCL!**) or combine it with a data frame to make a `phylo4d` (tree-with-data) object.

Now we'll take the *Geospiza* data from `geospiza_raw$data` and merge it with the tree. However, since *G. olivacea* is included in the tree but not in the data set, we will initially run into some trouble:

```
> g2 <- phylo4d(g1, geospiza_raw$data)
```

gives

```
Error in check_data(res, ...) :
  Tip data names are a subset of tree tip labels
(missing data names: platyspiza,pinaroloxias,olivacea)
(extra data names: Platyspiza,Pinaroloxias)
```

We have two problems — the first is that we forgot to lowercase the labels on the data to match the tip labels:

```
> gdata <- geospiza_raw$data
> row.names(gdata) <- tolower(row.names(gdata))
```

To deal with the second problem (missing data for *G. olivacea*), we have a few choices. The easiest is to use `missing.tip.data="OK"` to allow R to create the new object:

```
> g2 <- phylo4d(g1, gdata, missing.tip.data = "OK")
```

(setting `missing.tip.data` to `"warn"` would create the new object but print a warning).

Another way to deal with this would be to use `prune()` to drop the offending tip from the tree first:

```
> g1B <- prune(g1, "olivacea")
> phylo4d(g1B, gdata)
```

You can summarize the new object:

```
> summary(g2)

  No root edge.

 Phylogenetic tree : as(object, "phylo4")

 Number of tips    : 14
 Number of nodes   : 13
 Branch lengths:
        mean         : 0.1764008
        variance     : 0.04624379
        distribution :
   Min. 1st Qu.  Median 3rd Qu.    Max.
0.00917 0.04985 0.08000 0.21910 0.88080

Comparative data:

Tips: data.frame with 14 taxa and 5 variables

     wingL          tarsusL         culmenL          beakD
```

```
 Min.   :3.975   Min.   :2.807   Min.   :1.974   Min.   :1.191
 1st Qu.:4.189   1st Qu.:2.929   1st Qu.:2.187   1st Qu.:1.941
 Median :4.235   Median :2.980   Median :2.311   Median :2.073
 Mean   :4.236   Mean   :2.991   Mean   :2.333   Mean   :2.083
 3rd Qu.:4.265   3rd Qu.:3.039   3rd Qu.:2.430   3rd Qu.:2.347
 Max.   :4.420   Max.   :3.271   Max.   :2.725   Max.   :2.824
 NA's   :1.000   NA's   :1.000   NA's   :1.000   NA's   :1.000
     gonysW
 Min.   :1.401
 1st Qu.:1.845
 Median :1.962
 Mean   :2.014
 3rd Qu.:2.222
 Max.   :2.676
 NA's   :1.000

Object contains no node data.
```

Or use `tdata()` to extract the data (i.e., `tdata(g2)`). By default, `tdata()` will retrieve tip data, but you can also get internal node data only (`tdata(tree,"node")`) or — if the tip and node data have the same format — all the data combined (`tdata(tree,"allnode")`).

Plotting calls `plot.phylog` from the `ade4` package.

If you want to plot the data (e.g. for checking the input), `plot(tdata(g2))` will create the default plot for the data — in this case, since it is a data frame [**this may change in future versions but should remain transparent**] this will be a `pairs` plot of the data.

6 Subsetting

The `subset` command offers a variety of ways of extracting portions of a `phylo4` or `phylo4d` tree, keeping any tip/node data consistent.

tips.include give a vector of tips (names or numbers) to retain

tips.exclude give a vector of tips (names or numbers) to drop

mrca give a vector of node or tip names or numbers; extract the clade containing these taxa

node.subtree give a node (name or number); extract the subtree starting from this node

Different ways to extract the *fuliginosa-scandens* clade:

```
> subset(g2, tips.include = c("fuliginosa", "fortis", "magnirostris",
+     "conirostris", "scandens"))
```

```
> subset(g2, node.subtree = "N07")
> subset(g2, mrca = c("scandens", "fortis"))
```

One could drop the clade by doing

```
> subset(g2, tips.exclude = c("fuliginosa", "fortis", "magnirostris",
+     "conirostris", "scandens"))
> subset(g2, tips.exclude = names(descendants(g2, MRCA(g2, c("difficilis",
+     "fortis")))))
```

Another approach is to pick the subtree graphically, by plotting the tree and using `identify`, which returns the identify of the node you click on with the mouse.

```
> plot(g1)
> n1 <- identify(g1)
> subset(g2, node.subtree = n1)
```

7 Tree-walking

`getnodes`, `children`, `parent`, `descendants`, `ancestors`, `siblings`, `MRCA` ... generally take a `phylo4` object, a node (specified by number or name) and return a named vector of node numbers.

8 multiPhylo classes

9 Examples

9.1 Constructing a Brownian motion trait simulator

This section will describe two (?) ways of constructing a simulator that generates trait values for extant species (tips) given a tree with branch lengths, assuming a model of Brownian motion.

9.1.1 the easy way

We can use the `vcv.phylo()` command from `ape` to construct the variance-covariance matrix of the tip traits, after which it's easy to use `mvrnorm` from the `MASS` package to generate a set of multivariate normally distributed values for the tips. (A benefit of this approach is that we can very quickly generate a very large number of replicates.) This example illustrates a common feature of working with `phylobase` — combining tools from several different packages to operate on phylogenetic trees with data.

We start with a randomly generated tree using `rcoal()` from `ape` to generate the tree topology and branch lengths:

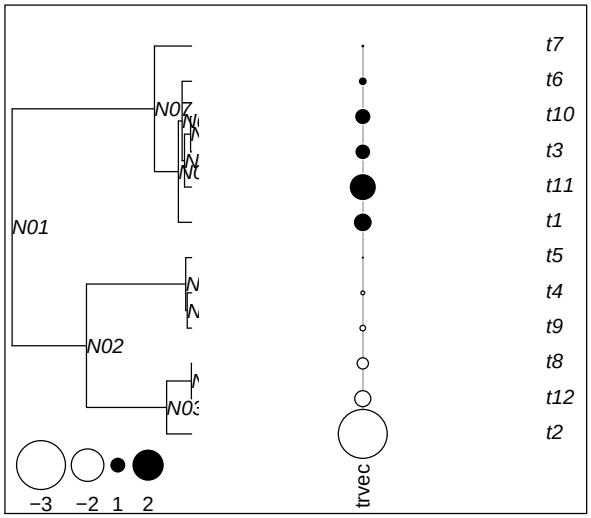
```
> set.seed(1001)
> tree <- rcoal(12)
```

Next we generate the phylogenetic variance-covariance matrix (`ape::vcv.phylo`) and pick a single set of traits (`MASS:mvrnorm`). Conveniently, the tip names of the original tree are inherited consistently by the variance-covariance matrix and the trait matrix:

```
> vmat <- vcv.phylo(tree, cor = TRUE)
> library(MASS)
> trvec <- mvrnorm(1, mu = rep(0, 12), Sigma = vmat)
```

The last step (easy) is to create the `phylo4d` object and plot it:

```
> treed <- phylo4d(tree, tip.data = as.data.frame(trvec))
> plot(treed)
```



9.1.2 The hard way?

Find root, traverse tree:

A Definitions/slots

This section details the internal structure of the `phylo4`, `multiphylo4`, `phylo4d`, and `multiphylo4d` classes. The basic building blocks of these classes are the `phylo4` object and a dataframe. The `phylo4` tree format is largely similar to the one used by `phylo` class in the package `ape` [1].

A.1 phylo4

Like `phylo`, the main components of the `phylo4` class are:

edge an $N \times 2$ matrix of integers, where the first column ...

edge.length numeric list of edge lengths (length N or empty)

Nnode integer, number of nodes

tip.label character vector of tip labels (required)

node.label character vector of node labels (maybe empty)

root.edge integer defining root edge (maybe NA)

We have defined basic methods for `phylo4`:`show`, `print` (copied from `print.phylo` in`ape`), and a variety of accessor functions (see help files). `summary` does not seem to be terribly useful in the context of a "raw" tree, because there is not much to compute: **end users?**

Print method: add information about (ultrametric, scaled, polytomies (zero-length or structural))?

A.2 phylo4d

The `phylo4d` class extends `phylo4` with data. Tip data, (internal) node data, and edge data are stored separately, but can be retrieved together or separately with `tdata(x,"tip")` or `tdata(x,"all")`.

edge data can also be included — is this useful/worth keeping?

A.3 multiphylo4

B Validity checking

- number of rows of edge matrix (N) == length of edge-length vector (if > 0)
- (number of tip labels)+(nNode)-1 == N
- data matrix must have row names

[1] http://ape.mpl.ird.fr/

- row names must match tip labels (if not, spit out mismatches)

Default node labels:

C Hacks/backward compatibility

There is a way to hack the `$` operator so that it would provide backward compatibility with code that is extracting internal elements of a `phylo4`. The basic recipe is:

```
> setMethod("$", "phylo4", function(x, name) {
+     attr(x, name)
+ })
```

but this has to be hacked slightly to intercept calls to elements that might be missing. For example, `ape` detects whether log-likelihood, root edges, node labels, etc. are missing by testing whether they are `NULL`, whereas missing items are represented in `phylo4` by zero-length vectors in the slots (or `NA` for the root edge) — so we need code like

```
> if (!hasNodeLabels(x)) NULL else x@node.label
```

to handle these cases.